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Title: Simulations of non-local spin interaction in atomic magnetometers using LANL's D-Wave 2X

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Simulations of non-local spin interaction in atomic magnetometers using LANL's D-Wave 2X

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4/27/2017

Nitrogen-vacancy (NV) defect in diamond

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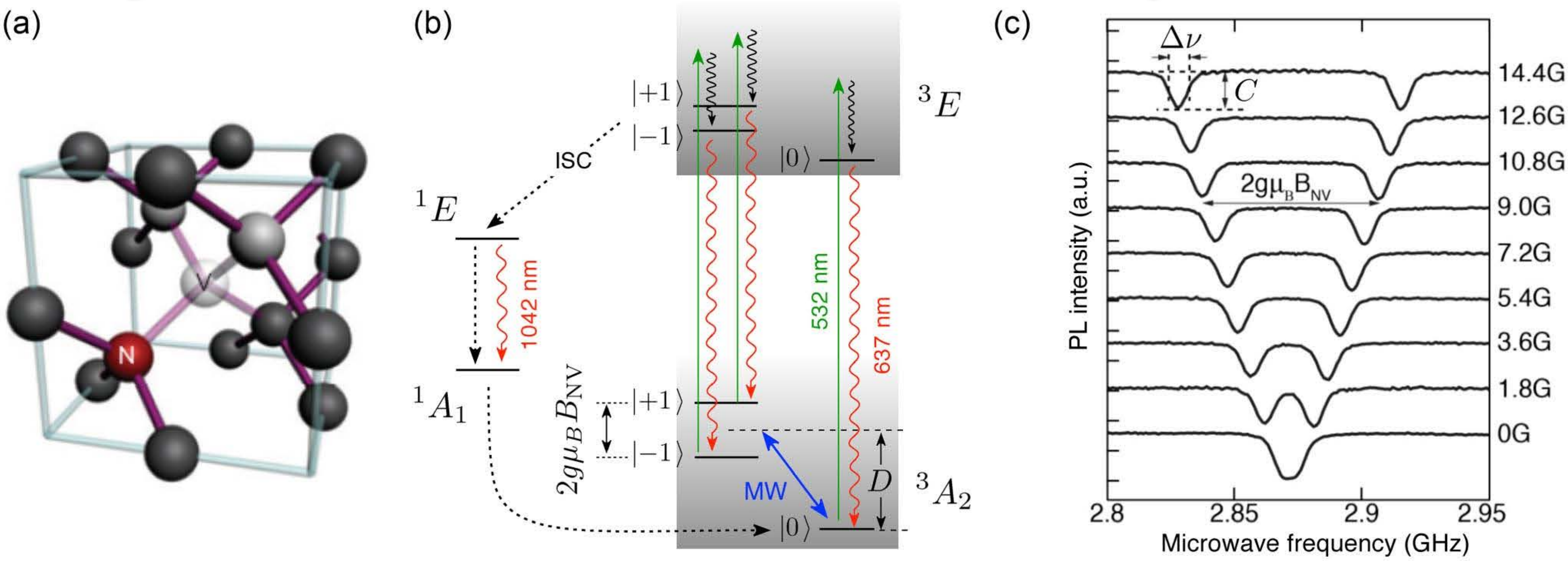
$$H = hDS_z{}^2 + hE\left(S_x{}^2 - S_y{}^2\right) + g\mu_B \boldsymbol{BS} + H_d$$



[1] Rep. Prog. Phys. **77** (2014) 056503 (26pp)

Simplifications of the Hamiltonian

D ~ 2.87 GHz or 100 mT

E ~ 100 kHz and can be neglected

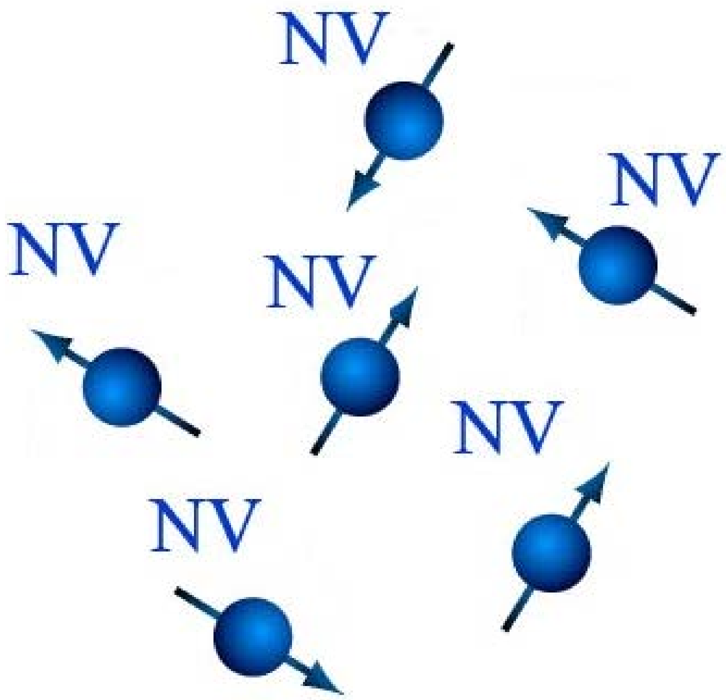
H_d ~ 100 mT for 1 nm, or 0.1 mT for 10 nm.

$hDS_z{}^2$ is not sensitive to the direction and does not play any role in our analysis when we consider only z component; however, forces the spin to be parallel to z.

Ensemble of NV defects:

Signal to noise ratio for independent NV-centers:

$$\boldsymbol{SNR} \sim \frac{\mathbf{1}}{\sqrt{\boldsymbol{N}}}$$



But dipole interaction between different NV-centers will also impact sensitivity and orientation of spins

$$H_i = -\sum \boldsymbol{m}_{NV\,i} \boldsymbol{B}_{NV\,j}$$

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A} = \frac{\mu_0}{4\pi}\left(\frac{3\mathbf{r}(\mathbf{m}\cdot\mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3}\right)$$

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Ising part of the Hamiltonian

Spin-spin interaction with random positioning is extremely hard problem for classical computer, but it ***seems to be an ideal fit for Ising Quantum Computer such as D-Wave***

Approximation: spin and magnetic field only along/opposite with z-axis; however, it can be justified for stationary states

$$H = \sum_i k_1 s_i B(r_i) + \sum_i \sum_{j<i} 2k_2 s_i s_j / r_{ij}^3 \left(1 - \frac{3z_{ij}^2}{r_{ij}^2}\right)$$

$$r_{ij} = \sqrt{(i_x - j_x)^2 + \left(i_y - j_y\right)^2 + (i_z - j_z)^2}; \; z_{ij} = (i_z - j_z)$$

Ground and excited states

To understand the dynamics of NV-diamond spins, the ground state is not sufficient and excited states also need to be found.

D-Wave finds automatically the ground state or low-excited states when the temperature is finite and the thermal energy is comparable to the splitting.

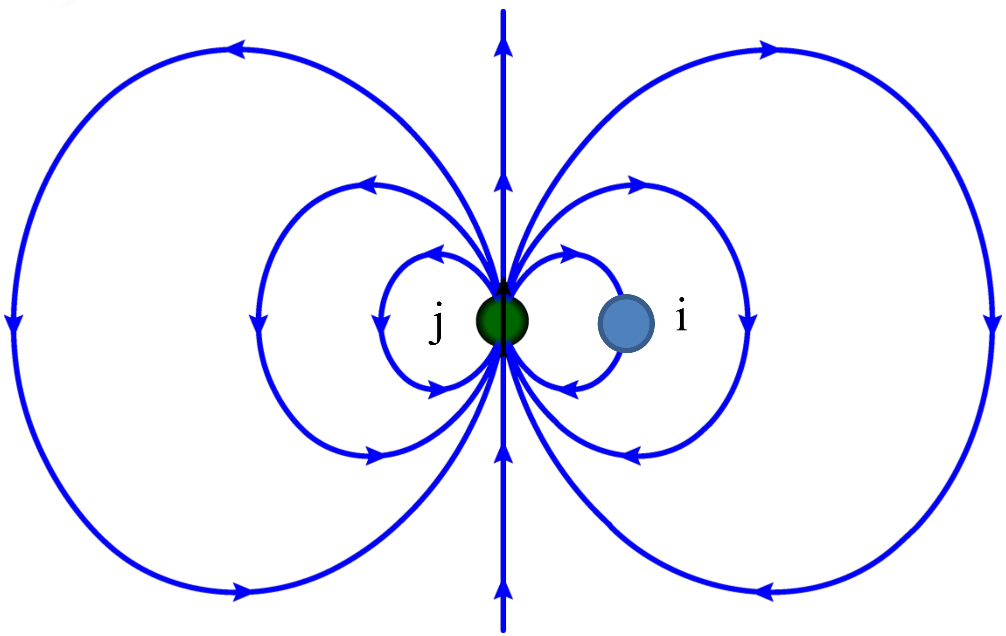
A more reliable method to find excited states is to introduce penalty energy for a state of being non-orthogonal to the ground state

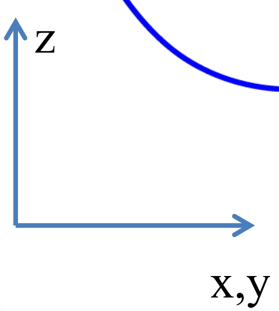
$$H = k_3 \sum_i s_i^{gr} s_i, \; k_3 > 0$$

This term can be combined with the Zeeman single-sum term and the new "ground" state, orthogonal to the real one is found by D-Wave. This process can be continued by adding the term enforcing orthogonality with the first excited states, and so on.

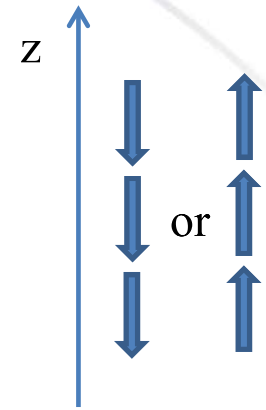
Dipole field map to predict solutions

We can predict solutions in some trivial spin configurations



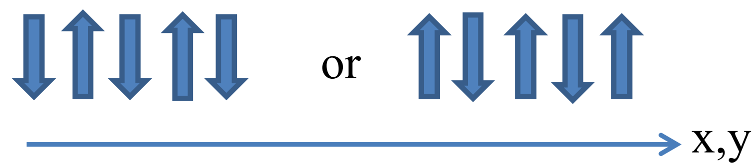


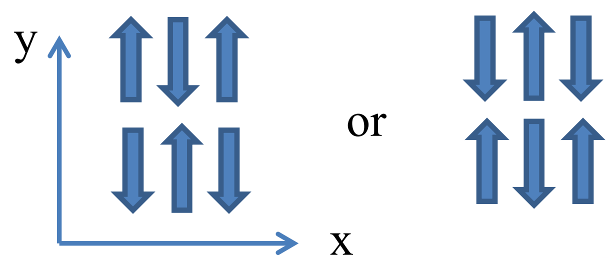
No external magnetic field :
2x degenerate ground level



$H_d = -\boldsymbol{m}_i \boldsymbol{B}_j$:

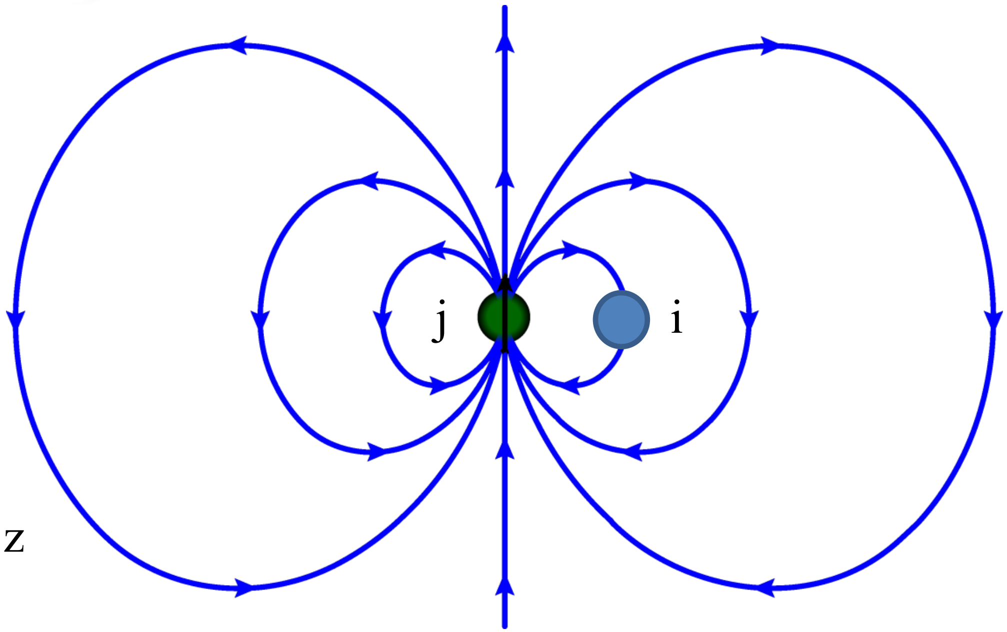
Spin is aligned with magnetic field of its closest neighbor to minimize Hamiltonian

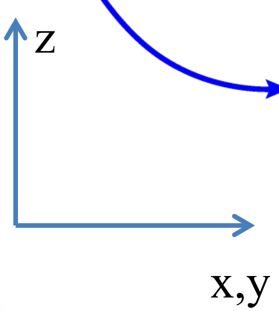




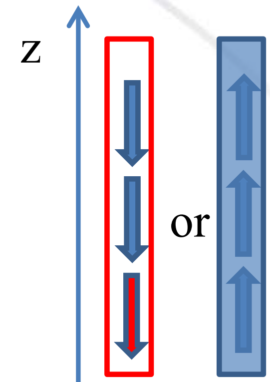
Dipole field map to predict solutions

We can predict solutions in some trivial spin configurations



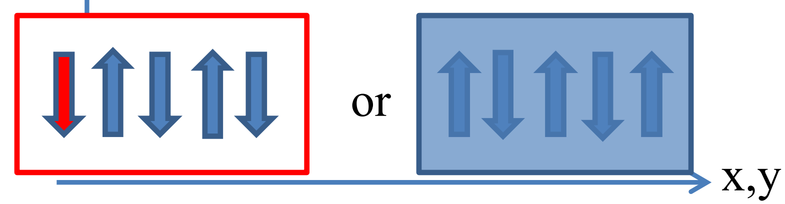


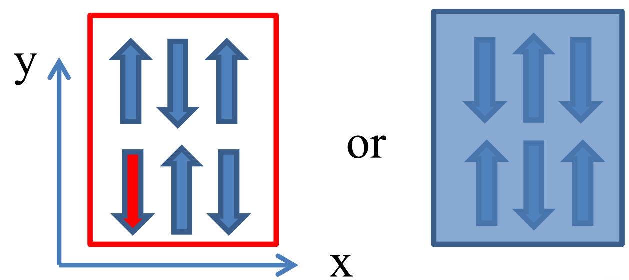
First spin is fixed down by strong magnetic field: selecting one solution



H= $-\boldsymbol{m}_i\boldsymbol{B}_j$:

spins are aligned with magnetic field to minimize Hamiltonian:





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Is D-Wave 2X capable to find energy levels (*at least ground state*) of many (*how many?)* NV-diamond spins system in our approximation?

Problems we found

1. **D-Wave 2X bias:** spin up and spin down are not the same

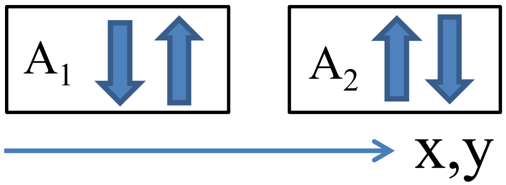
2. Embedding:

a) increasing the number of spins in the system requires a lot of couplings, which squeezes the dynamic range

b) only 45 spins connected to each other are possible to simulate on D-Wave 2X unless we “cheat” and cut long distance interaction

2-spin system (x/y-line): no embedding needed

Expectations:
50% and 50%



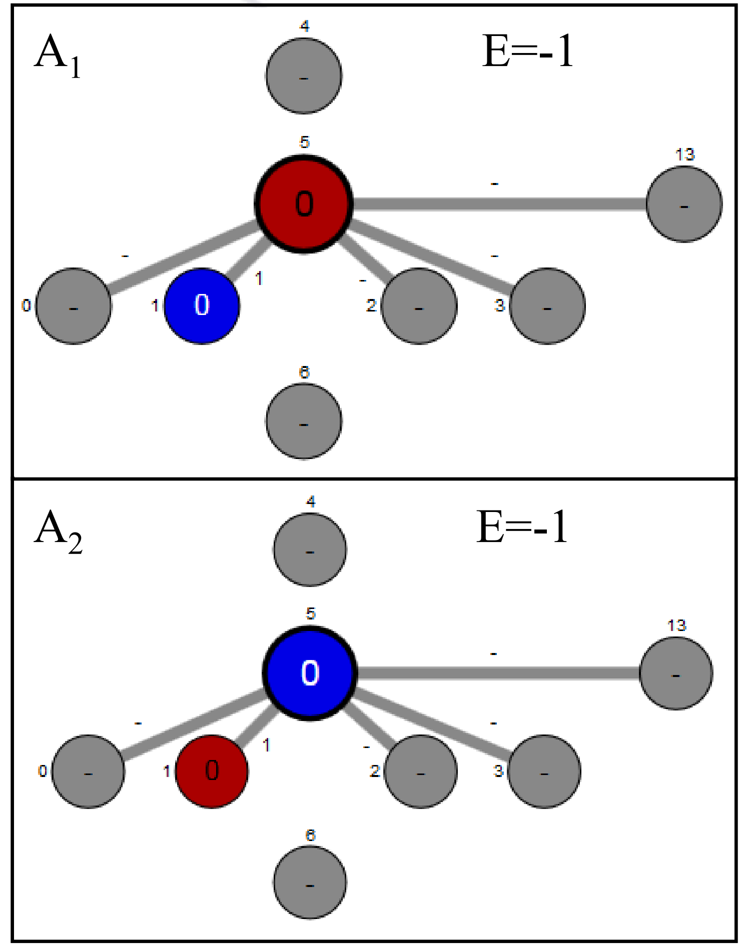
Samples=1000

Run	1	2	3	4	5	Total
A_1	565	570	474	612	440	2661
A_2	435	430	526	388	560	2339

Classical computer states to compute E and sort*: $n=2^2=4$

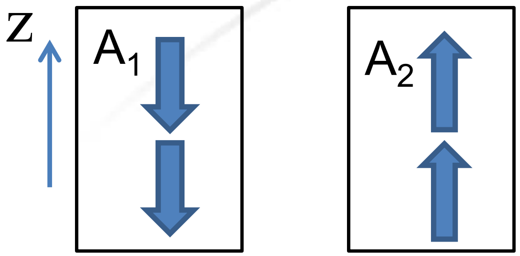
Quick sort:
$D_{min}=n\log(n)$
$D_{max}=n^2$

D-Wave solutions:

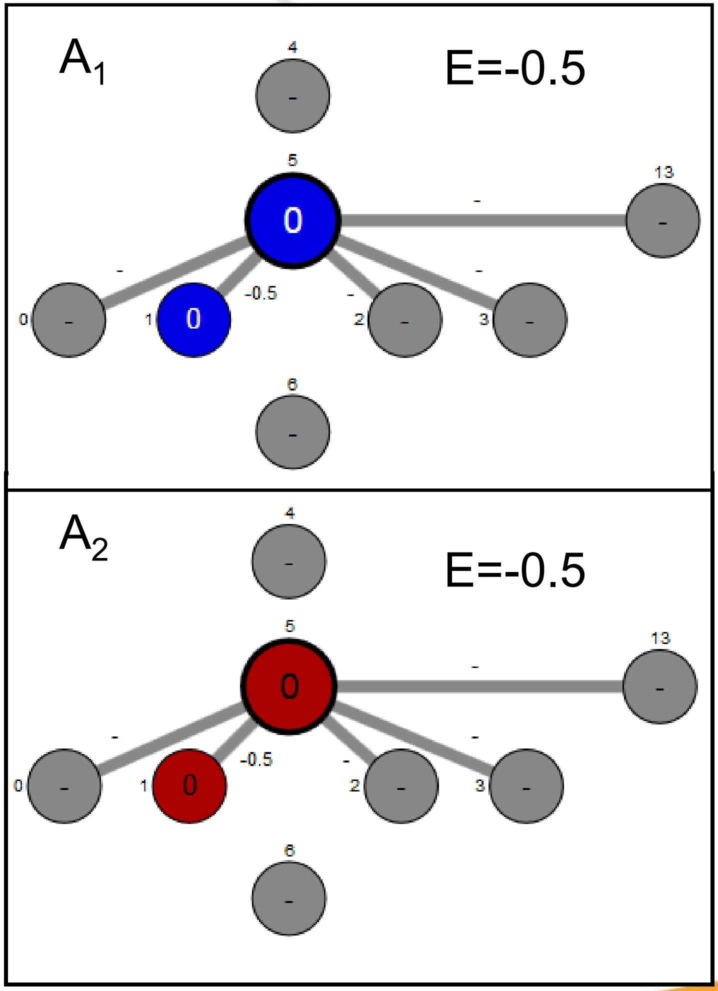


2-spin system (z-line): no embedding needed

Expectations:
50% and 50%



D-Wave solutions:



Samples=1000;

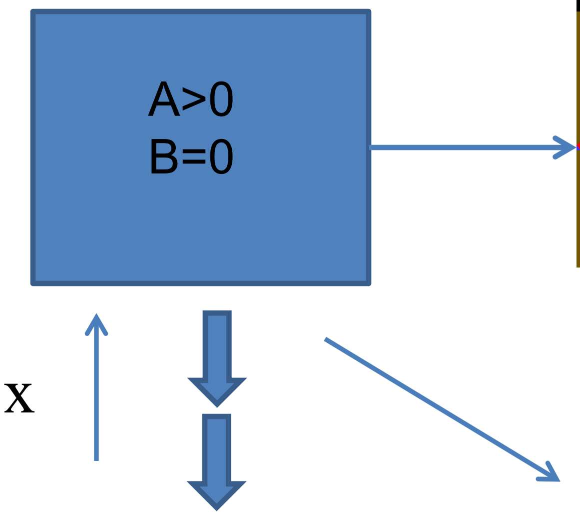
Bias?

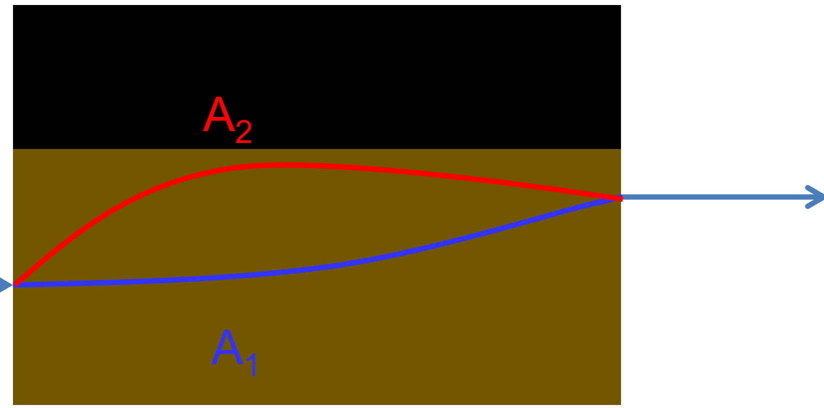
Run	1	2	3	4	5	Total
A_1	714	626	683	755	658	3436
A_2	286	374	317	245	342	1564

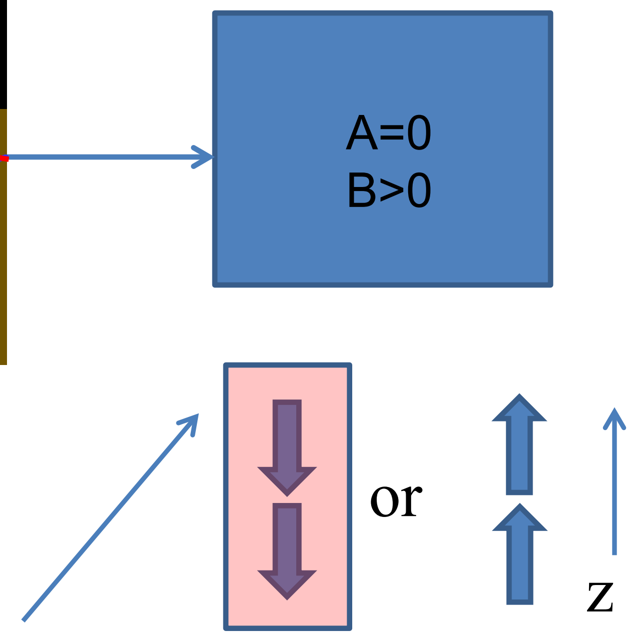
Bias: adiabatic DWAVE evolution

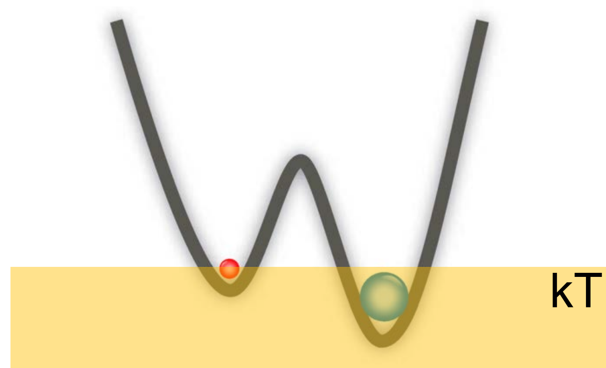
$$E_{ising}(s) = \frac{A(s)}{2}\left(\sum_i \sigma_x^{(i)}\right) + \frac{B(s)}{2}\left(\sum_i h_i \sigma_z^{(i)} + \sum_{i>j} J_{i,j}\sigma_z^{(i)}\sigma_z^{(j)}\right)$$

Bias dependence from temperature (annealing time) will be an interesting problem to study





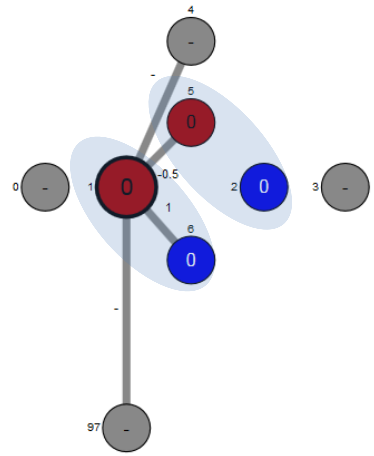




What is the evolution path: A$(S)-?\ B(S)-?$

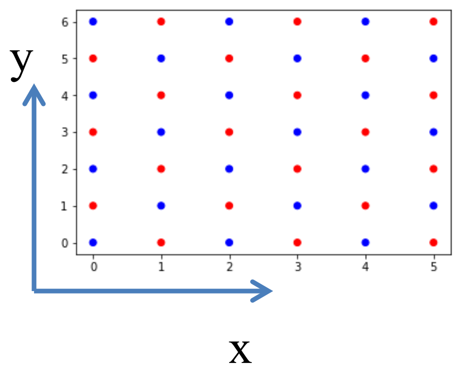
How to get right solutions with biased D-Wave

1. Spin anti-cloning
*Problem: squeezing dynamic range **



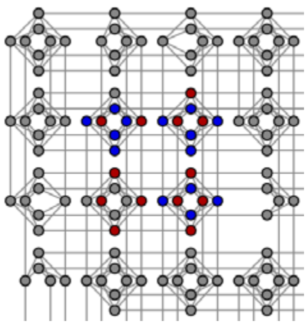
Anti-cloning based embedding would be ideal for systems which need embedding anyway
**dynamic range would be the same as in regular embedding*

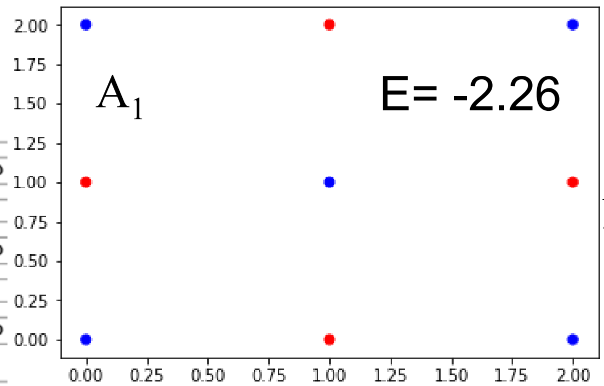
2. Choosing symmetrical relatively to spin direction systems to study

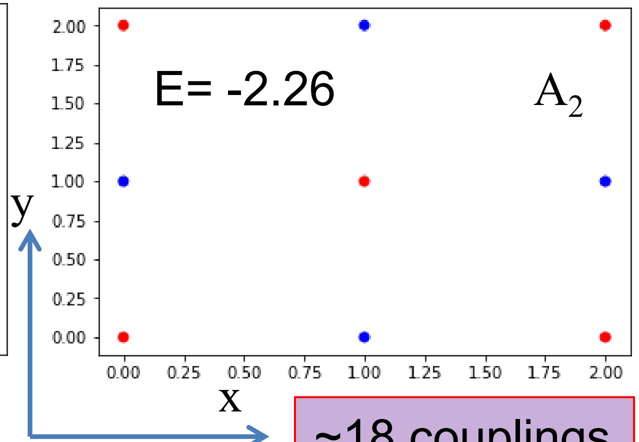


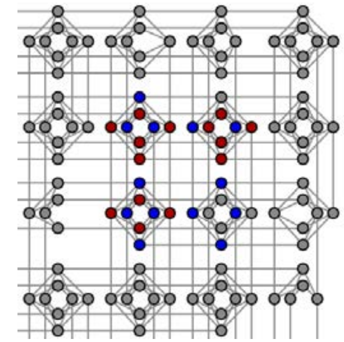
For such symmetrical systems all embedding chains should be ideally of the same length

2D spin system: 9=3*3 spins



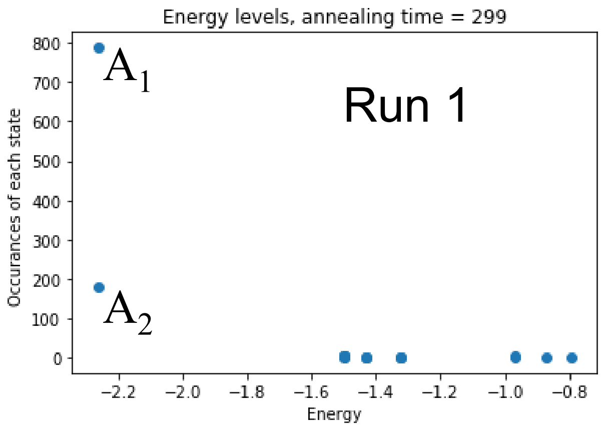


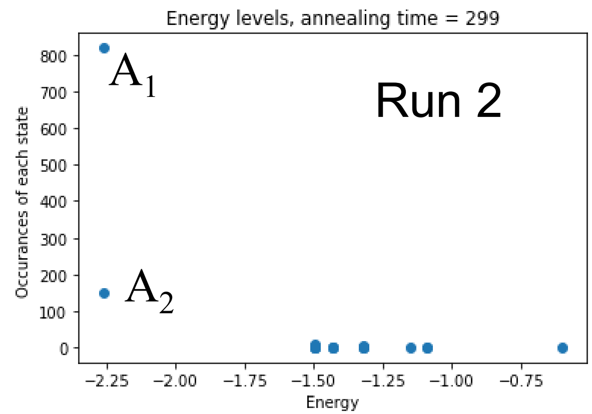


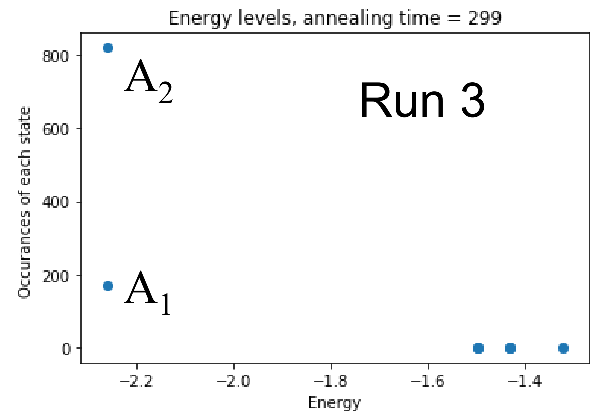


Samples=1000

~18 couplings







Classical computer states to compute E and sort*: $n=2^9=512$

*Quick sort: $D_{min}=n\log(n)$, $D_{max}=n^2$

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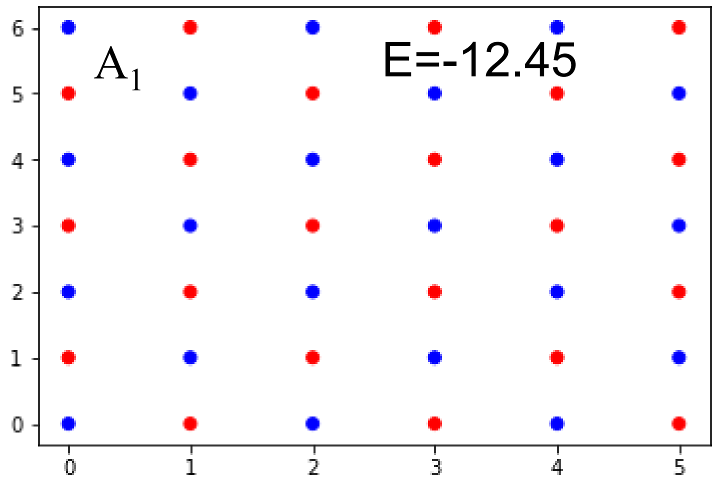
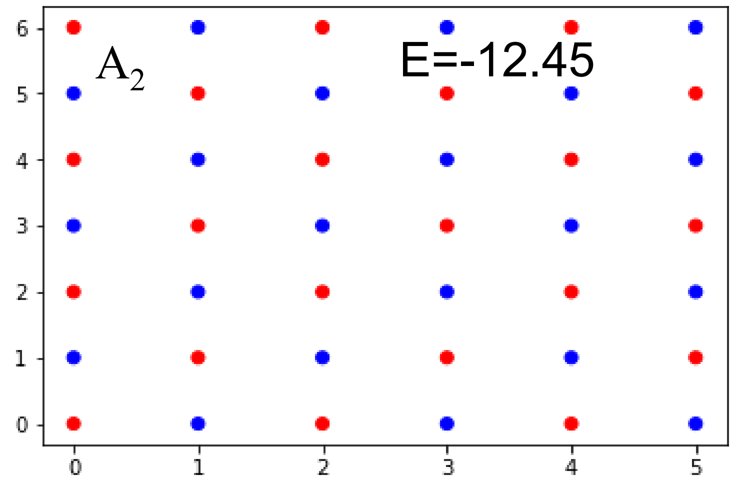
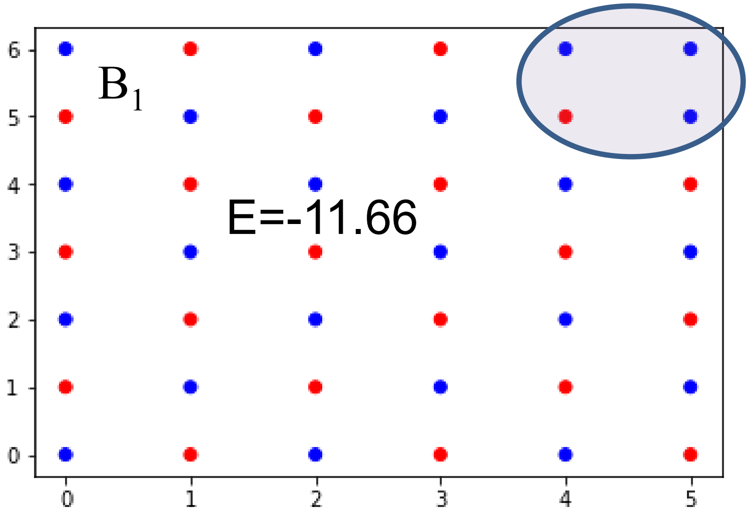
2D spin system: 42=6*7 spins







Spin flip

~800 couplings

Classical computer states to compute E and sort*: $n=2^{42} \sim 4*10^{12}$

**Quick sort:*
$D_{min}=n\ log(n)$
$D_{max}=n^2$

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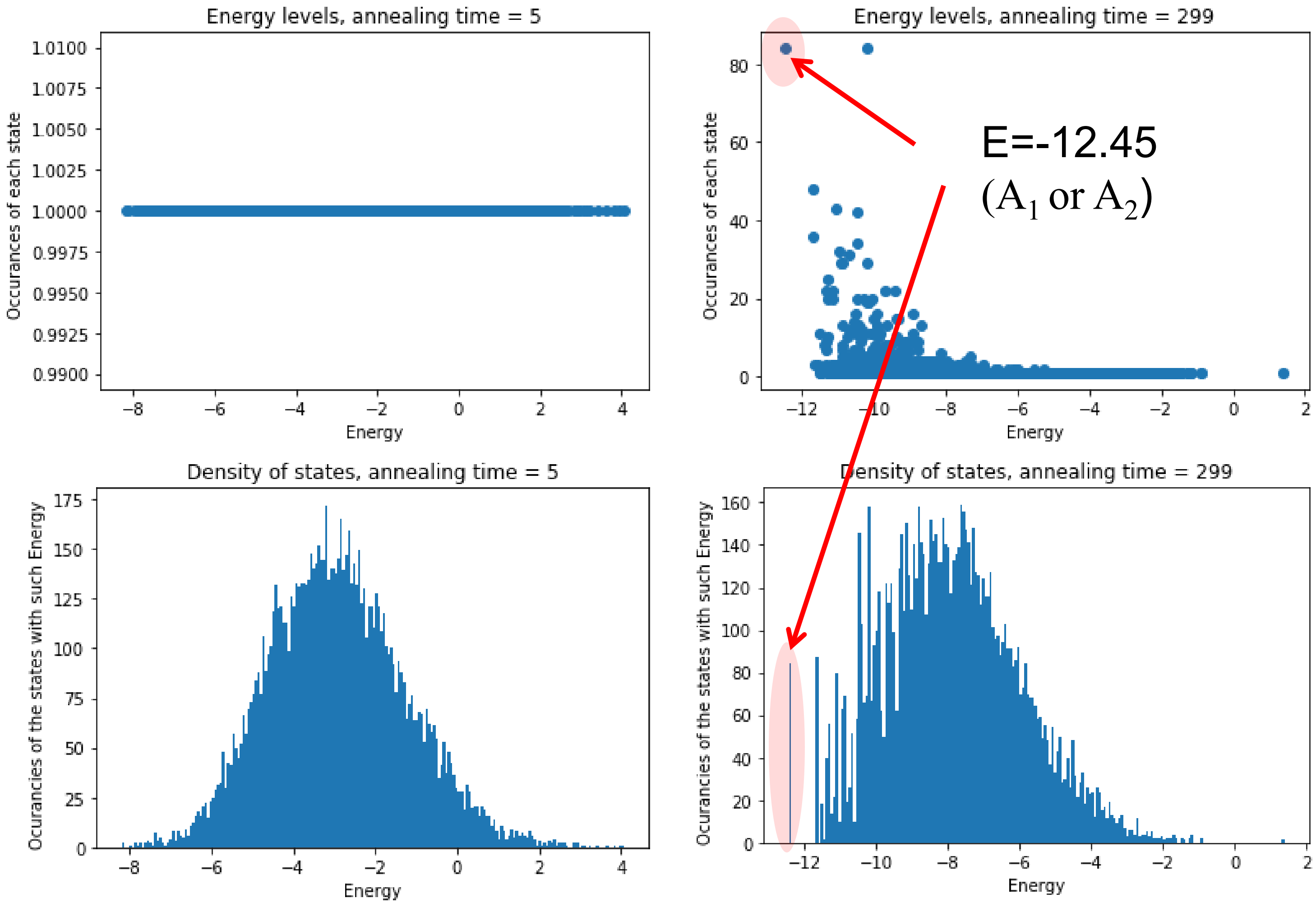
Annealing time dependence

42 spins, samples=10000



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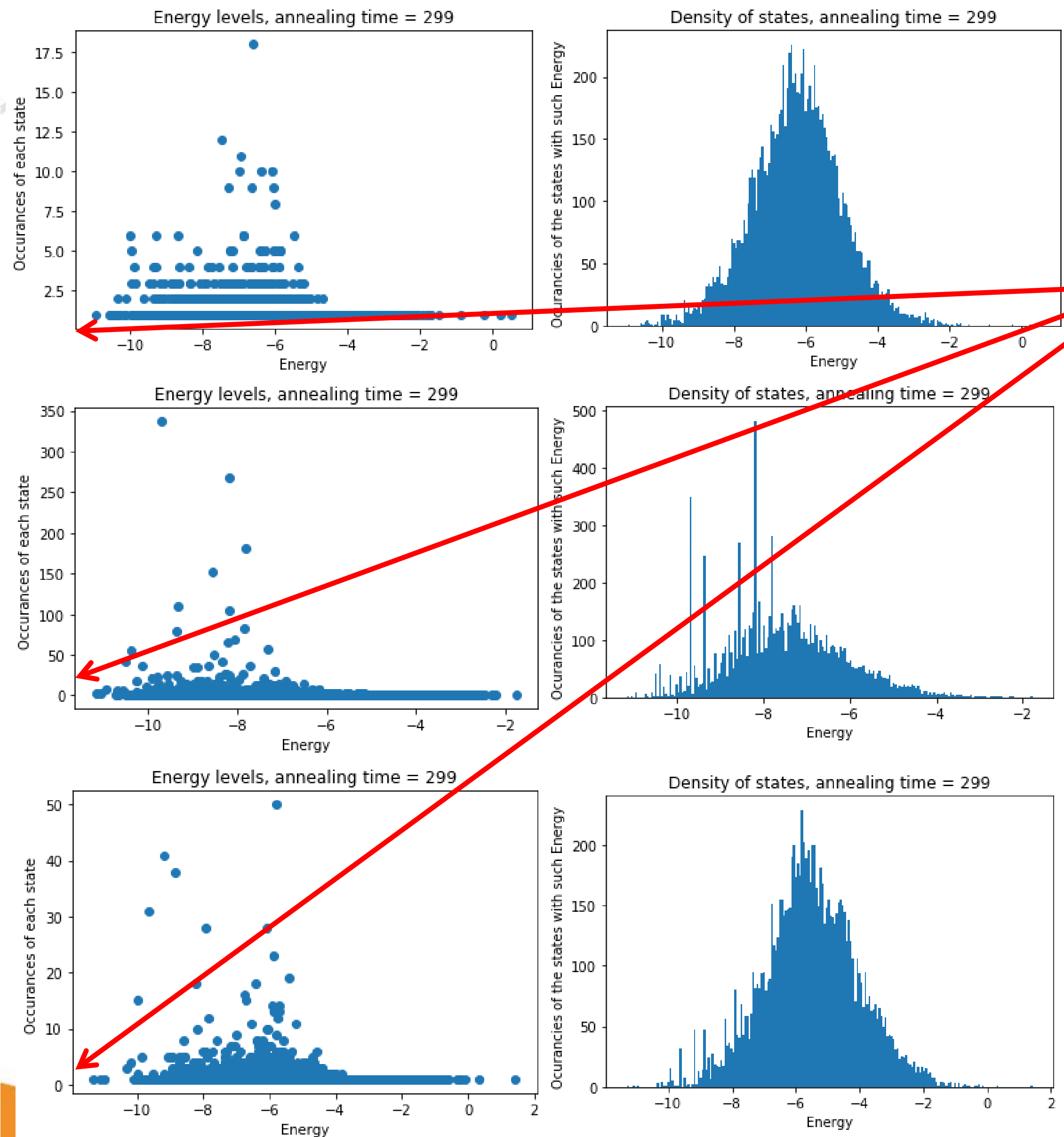
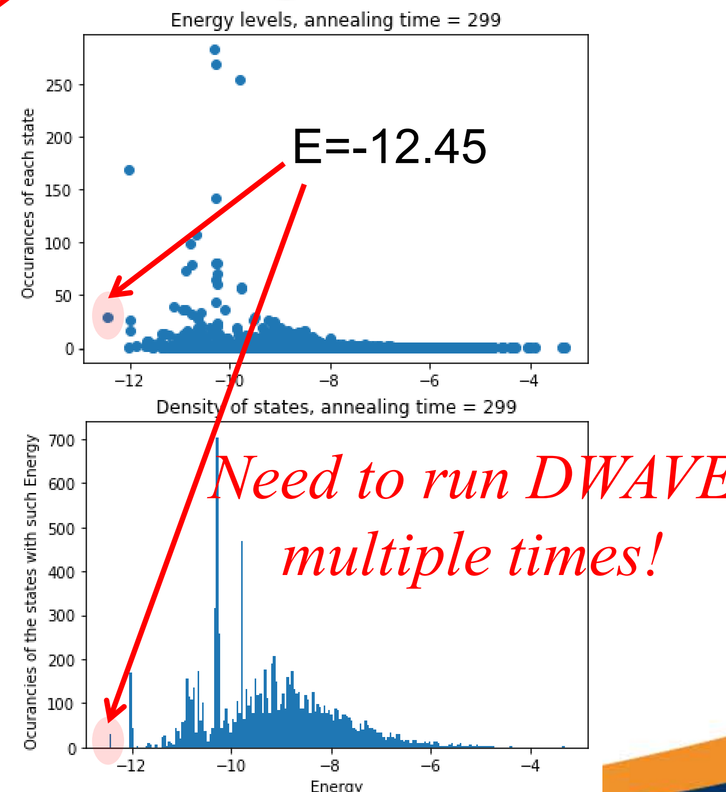
Same parameters – different results

Missing ground level solution 3 times from 4



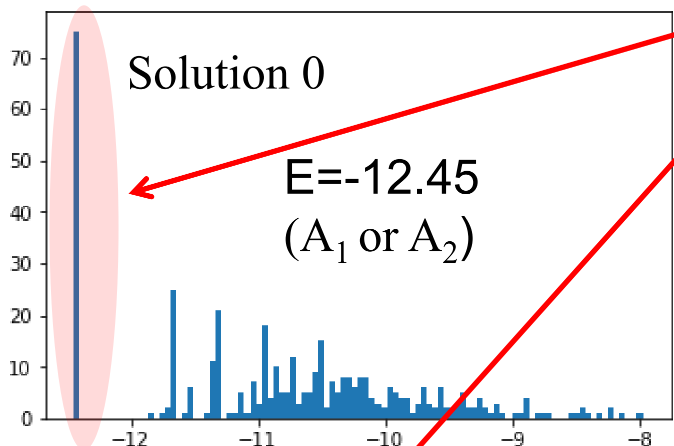


Annealing time dependence: multiple runs

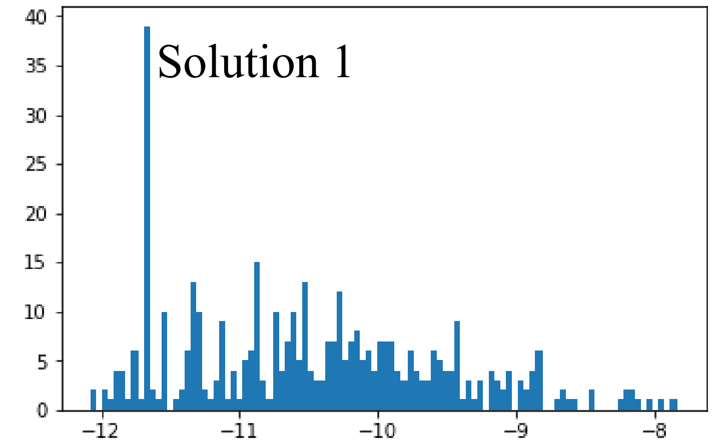
Only analyzing two first (lowest energy) levels from DWAVE each run:

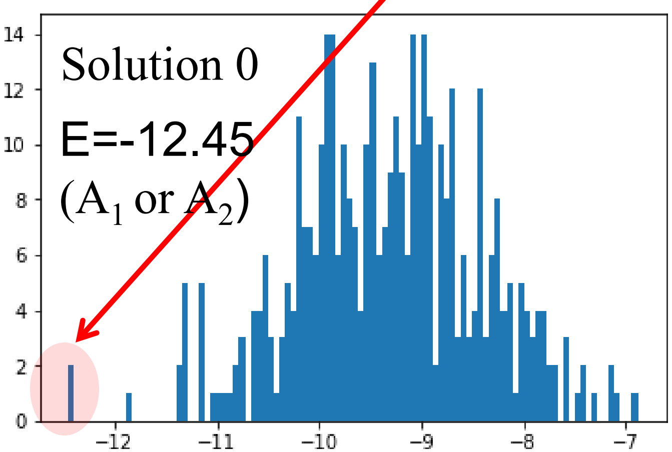
[runs=400, samples=10000]

Solution 0 and 1 should have the same energy ~-12.45, but we find only "0" in ground state

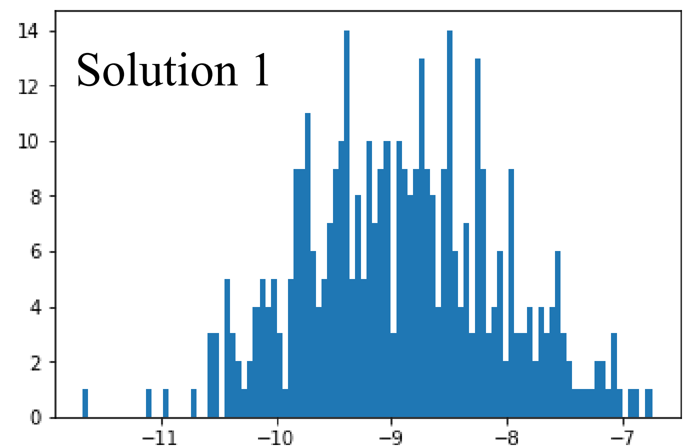


Annealing time = 299





Annealing time = 5



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